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TR-1779—RARE EARTH ION-HOST LATTICE INTERACTIONS
by Clyde A. Morrison, Donald E. Wortman, and Nick Karayianis

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RARE EARTH ION-HOST LATTICE INTERACTIONS

14. Lanthanide Pentaphosphates

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7.61 cm⁻¹, a fit of 10.43 cm⁻¹ to 46 Eu³⁺ levels is obtained. Predicted B_{km} and energy levels for all the lanthanide pentaphosphates are then obtained.

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1. INTRODUCTION

Interest in new materials that have potentially good laser properties has recently been focused on the rare-earth pentaphosphates.¹ The apparent lack of quenching between the active ions in these materials, as evidenced by the sharp lines observed even when there is 100-percent doping as in NdP₅O₁₄, leads to the obvious expectation of producing smaller laser crystals with these materials.

In this work, previously reported spectra of the pentaphosphates of Nd and Eu were analyzed by diagonalizing a parametrized $C_s(C_{1h})$ Hamiltonian in free-ion bases involving the five and seven lowest J-multiplets, respectively, of each ion. By reassigning symmetries to the reported² Eu levels according to predictions from scaled crystal field parameters, B_{km} , that fit 28 Nd levels³ to 7.61 cm^{-1} , a fit of 10.43 cm^{-1} to 46 levels of Eu was obtained. Predicted B_{km} and energy levels for all the lanthanide pentaphosphates also were obtained.

2. CALCULATIONS

The point group symmetry at the rare-earth ion site^{4,5} is C_1 which gives rise to the crystal field Hamiltonian

¹H. G. Danielmeyer and H. P. Weber, *IEEE J. Quantum Electron.*, QE-8 (1972), 805.

²C. Brecher, *J. Chem. Phys.*, 61 (1974), 2297.

³M. Blatte, H. G. Danielmeyer, and R. Ulrich, *Appl. Phys.*, 1 (1973), 275.

⁴H. Y-P Hong, *Acta Crystallogr.*, B30 (1974), 468.

⁵K.-R. Albrand, R. Attig, J. Fenner, J. P. Jeser, and D. Mootz, *Mater. Res. Bull.*, 9 (1974), 129.

$$H_x = \sum_{km} B_{km} C_{km}, \quad k = 2, 4, 6, \quad (1)$$

where $|m| \leq k$ and B_{km} for $m \neq 0$ may be complex. This Hamiltonian represents the lowest possible symmetry in the electrostatic potential at the rare-earth site, and it contains 26 independent B_{km} , counting real and imaginary parts of the B_{km} . In order to obtain a manageable representation for the crystal field that may be extended to predict spectra of all the lanthanide pentaphosphates, we assume the B_{km} with $m = \pm$ odd integer to be negligible (subject to justification at a later date). The resulting Hamiltonian given by equation (1) with the added restriction

$$m = 0, \pm 2, \dots, \pm k \quad (2)$$

results in 14 independent parameters and has the appearance of C_s (C_{1h}) symmetry.

This Hamiltonian was diagonalized in free-ion bases by using the lowest five and seven J-multiplets, respectively, of Nd and Eu, and the B_{km} and multiplet centroids were varied to fit reported spectra for $\text{NdP}_5\text{O}_{14}$ ³ and $\text{EuP}_5\text{O}_{14}$.² To begin the analysis, the B_{km} of Brecher² were converted from the form⁶ $A_k^m \langle r^k \rangle$ to the B_{km} of equation (1). These B_{km} , given in table I, line 1, were then used to calculate theoretical energy levels for the 7F term of Eu. Crystal quantum numbers $\mu = 0, 1$ were assigned to experimental energy levels according to which theoretical level each approximated. By maintaining these assignments, the B_{km} and

²C. Brecher, *J. Chem. Phys.*, 61 (1974), 2297.

³M. Blatte, H. G. Danielmeyer, and R. Ulrich, *Appl. Phys.*, 1 (1973), 275.

⁶A. J. Kassman, *J. Chem. Phys.*, 53 (1970), 4118.

centroids were varied to give a best fit of 14.6 cm^{-1} for 49 levels with the B_{km} of table I, line 2. These B_{km} were then scaled according to the ratios⁷

$$B_{km}(\text{Nd})/B_{km}(\text{Eu}) = 1.024, 1.194, 1.271; k = 2, 4, 6, \quad (3)$$

and used as starting parameters to fit the 28 levels of the ^4I term and $^4\text{F}_{3/2}$ multiplet of Nd. A fit of 7.6 cm^{-1} was obtained with the B_{km} of table I, line 4.

Since the final B_{km} for Nd differed significantly from the initial set, they were then scaled back to Eu to determine if new crystal quantum number assignments to the Eu levels would result in a better fit. By maintaining the new assignments, a second set of B_{km} given in table I, line 3, was obtained that gave a fit of 13.2 cm^{-1} , better than the 14.6 cm^{-1} resulting from Brecher's assignments, but not as good a fit as the Nd spectrum. Three experimental levels at 1928, 4952, and 4993 cm^{-1} differed by more than 30 cm^{-1} from theoretical values in the best-fit calculation for Eu. If they are ignored, the 13.2-cm^{-1} fit for 49 levels is reduced to a 10.4-cm^{-1} fit without any further refitting of the B_{km} to the remaining 46 levels.

Comparing the final parameters for Eu in table I, line 3, with those of Nd in line 4, it is not clear what the best way is of extending the results to all the lanthanides. There is some consistency between the parameters, however, if one compares the rotational invariants $B_{oo}(k, N)$ for each ion where we define⁸

$$B_{oo}(k, N) = \left[\sum_m |B_{km}(N)|^2 \right]^{1/2}, \quad (4)$$

⁷N. Karayianis, D. E. Wortman, and C. A. Morrison, *Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate, Solid State Communications* 18 (1976), 1299.

⁸N. Karayianis, C. A. Morrison, and D. E. Wortman, *J. Chem. Phys.*, 64 (1976), 3890.

TABLE I. CRYSTAL FIELD PARAMETERS, B_{km} , IN CM⁻¹ FOR NdP₅O₁₄ AND EuP₅O₁₄

Ion	B_{20}	B_{22}	B_{40}	B_{42}		B_{14}		B_{60}		B_{62}		B_{64}		B_{66}		Multiplets (No.)	Experimental levels (No.)	Experimental rms deviation (cm ⁻¹)
				Real	Imaginary													
Eu ^a	-508	167	648	146	0	-847	0	195	74	0	75	0	-401	0	7	49	49	18.94
Eu ^b	-453	270	720	114	100	-799	49	245	97	-41	-22	-257	-424	-16	7	49	49	14.56
Eu ^c	-586	213	-83	751	80	111	-184	132	-118	388	81	-68	-457	-3	7	40	49	13.18
Nd ^d	-785	16	-219	-661	149	-621	52	291	-242	-275	249	-391	18	-176	5	28	28	10.43
																		7.61

^aBrecher's parameters with J-mixing included and centroids adjusted for best rms fit (C. Brecher, J. Chem. Phys., 61 (1974), 2297).

^bBest B_{km} fitting levels with crystal quantum number assignments from calculation of line 1.

^cBest B_{km} fitting levels with crystal quantum number assignments starting with B_{km} scaled from line 4.

^dBest B_{km} starting with B_{km} scaled from line 2.

and N represents the configuration f^N of the particular lanthanide. Table II gives the quantities $B_{\infty}(k, 3)$ and $B_{\infty}(k, 6)$ calculated for Nd and Eu, respectively, by using their final B_{km} values from table I. These quantities tend toward lower values as N gets larger. To derive B_{km} for all the lanthanides, we defined⁸ average constants η_{km} independent of N by

$$\eta_{km} = \frac{1}{2} \left[\frac{|B_{km}(Nd)|}{B_{\infty}(k, 3)} + \frac{|B_{km}(Eu)|}{B_{\infty}(k, 6)} \right], \quad (5)$$

chose expressions for the $B_{\infty}(k, N)$ and phases $\phi_{km}(N)$ linear in N^* to fit the values in tables II and I, respectively, and calculated B_{km} for all the lanthanides by

$$B_{km}(N) = \eta_{km} B_{\infty}(k, N) \exp[i\phi_{km}(N)]. \quad (6)$$

The parameters given by equation (6) were reported elsewhere.⁸ A simpler method was used here, however, to obtain the B_{km} for the lanthanides. This method consists of deriving a set of B_{km} such that

$$B_{km}(N) = B_{km}(x) + \rho_k(N)/\rho_k(x) \quad (7)$$

for $x = \text{Nd}$ and then for $x = \text{Eu}$; the ρ_k are from table II by Karayianis et al.⁷ The resulting B_{km} were then averaged, and these parameters are given in table III.

^{*} N is the number of equivalent 4f electrons specifying the electronic configuration for that ion. $N = 2$ for Pr, 3 for Nd, etc.

⁷N. Karayianis, D. E. Wortman, and C. A. Morrison, Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate, Solid State Communications 18 (1976), 1299.

⁸N. Karayianis, C. A. Morrison, and D. E. Wortman, J. Chem. Phys., 64 (1976), 3890.

TABLE II. ROTATIONAL INVARIANTS $B_{OO}(k, N) = (\sum_m |B_{km}(N)|^2)^{1/2}$ FOR $\text{NdP}_5\text{O}_{14}$ AND $\text{EuP}_5\text{O}_{14}$

k	Nd	Eu
	$B_{OO}(k, 3)^a$	$B_{OO}(k, 6)^b$
2	785	659
4	1320	1114
6	920	887

^aCalculated from table I,
line 4.

^bCalculated from table I,
line 3.

Energy levels calculated by using the B_{km} of tables I and III for the lowest-lying six to eight multiplets of the lanthanide pentaphosphates are given in tables IV to XVI.

In order to make intensity calculations, some estimates of the odd-fold (odd-k) crystal field components (A_{km}) are necessary. These can be obtained by appropriate lattice sums.⁹ In this work, we have performed the lattice sums for $\text{NdP}_5\text{O}_{14}$ using the x-ray data of Hong⁴ for oxygen charges $q_0 = -1$ and -2 ; the results are given in table XVII. The one fold field, A_{1m} , is not expected to be accurate because of its slow convergence. By appropriate rotations of the coordinate system chosen for the calculation of the A_{km} of table XVII, different sets of A_{km} can be generated. Since the A_{km} are linear functions of q_0 , a value of q_0

can be chosen by using the relation $B_{km} = \rho_k A_{km}$ and the ρ_k (reported in table II by Karayianis⁷) to obtain a best fit of calculated B_{km} to phenomenological B_{km} .

⁴H. Y-P Hong, *Acta Crystallogr.*, B30 (1974), 468.

⁷N. Karayianis, D. E. Wortman, and C. A. Morrison, *Crystal Field Parameters for Triply Ionized Lanthanides in Yttrium Orthoaluminate, Solid State Communications* 18(1976), 1299.

⁹N. Karayianis and C. A. Morrison, *Rare Earth Ion-Host Lattice Interactions 1. Point Charge Lattice Sum in Scheelites, Harry Diamond Laboratories TR-1648 (October 1973)*.

TABLE III. ESTIMATED CRYSTAL FIELD PARAMETERS, B_{km} , IN cm^{-1} FOR LnP_{214} SPACE GROUP
 $P_{21/c}^{\overline{c}}$) WHERE Ln IS ONE OF THE LANTHANIDES

Ion	B_{20}	B_{22}	B_{40}	B_{42}		B_{44}		B_{60}		B_{62}		B_{64}		B_{66}		Table No.
				Real	Imaginary											
Pr	-780	158	-164	-621	-536	-152	-474	240	-338	205	156	-312	210	-301	-	IV
Nd	-755	153	-159	-773	174	-479	40	235	-256	-290	183	-288	36	-357	9.739 ^a	V
Pm	-729	148	-153	-307	698	-66	459	230	236	-295	208	-261	-139	-322	-	VI
Sm	-703	142	-147	364	636	415	160	224	324	176	228	-232	-272	-209	-	VII
Eu	-675	137	-140	696	82	238	-353	218	-114	341	245	-202	-330	-49	b	X
Gd	-646	131	-134	457	-487	-277	-296	213	-346	-52	258	-171	-304	115	-	XI
Tb	-616	125	-127	-114	-623	-332	193	207	-9	-340	267	-139	-204	242	-	XII
Dy ^c	-584	118	-119	-535	-262	107	346	201	324	-66	271	-107	-59	301	-	XIII
Ho ^c	-551	112	-111	-494	257	337	-25	194	118	297	272	-76	92	283	-	XIV
Er ^c	-515	104	-103	-81	508	47	-308	188	-263	162	269	-45	211	195	-	XV
Tm ^c	-477	97	-94	328	334	-264	-105	181	-198	-222	263	-16	269	65	-	XVI

^aFit to data of C. Brecher, J. Chem. Phys., 61 (1974), 2297.

^bFit to data of table I, lines 1 and 2.

^cThese lanthanides have not been grown in the $P_{21/c}$ space group structure.

TABLE IV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{PrP}_5\text{O}_{14}$

PR IN PRP5O14. EXTERPOLATED BKM FROM COMPATIBLE NO AND EU HMF'S. 9/24/75.					
INIT. BKM AND CENTRIDS. Q = -0.000					
-779.700	= 820	158.100	= 822	-164.300	= 840
240.100	= 860	-337.700	= 862	205.400	= 862
3H 4	251.0				
3H 5	2354.4	-151.600	= 844	-474.500	= 844
3H 6	4527.0	210.500	= 866	-300.900	= 866
3F 2	5101.0				
3F 3	6478.0				
3F 4	6950.0				
1G 4	9923.0				
10 2	16802.0				
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY	
1 3H 4	99.6	2	-65.1	0.0	
2 3H 4	99.3	0	-14.6	0.0	
3 3H 4	99.5	0	70.4	0.0	
4 3H 4	99.4	2	203.3	0.0	
5 3H 4	99.5	2	249.6	0.0	
6 3H 4	99.5	0	305.3	0.0	
7 3H 4	99.6	2	333.9	0.0	
8 3H 4	99.2	0	489.7	0.0	
9 3H 4	99.5	0	523.4	0.0	
10 3H 5	99.1	2	2077.1	0.0	
11 3H 5	99.0	0	2085.7	0.0	
12 3H 5	98.7	0	2189.9	0.0	
13 3H 5	98.7	2	2238.3	0.0	
14 3H 5	99.1	2	2295.7	0.0	
15 3H 5	99.0	0	2387.1	0.0	
16 3H 5	99.2	2	2397.7	0.0	
17 3H 5	98.7	0	2407.4	0.0	
18 3H 5	99.2	0	2440.9	0.0	
19 3H 5	98.8	2	2598.7	0.0	
20 3H 5	99.4	2	2617.1	0.0	
21 3H 6	98.7	2	4177.9	0.0	
22 3H 6	98.9	0	4178.3	0.0	
23 3H 6	97.7	0	4310.5	0.0	
24 3H 6	98.4	2	4351.9	0.0	
25 3H 6	98.7	2	4416.8	0.0	
26 3H 6	98.4	0	4484.4	0.0	
27 3H 6	98.2	0	4515.7	0.0	
28 3H 6	97.1	2	4590.2	0.0	
29 3H 6	98.1	0	4617.2	0.0	
30 3H 6	98.5	2	4631.3	0.0	
31 3H 6	97.6	2	4667.8	0.0	
32 3H 6	92.2	0	4812.9	0.0	
33 3H 6	95.8	0	4829.7	0.0	
34 3F 2	94.5	0	5060.7	0.0	
35 3F 2	97.1	0	5070.0	0.0	
36 3F 2	96.7	2	5146.3	0.0	
37 3F 2	97.2	2	5172.2	0.0	
38 3F 2	92.9	0	5220.3	0.0	
39 3F 3	96.1	2	6402.9	0.0	
40 3F 3	98.3	2	6445.1	0.0	
41 3F 3	96.0	0	6474.1	0.0	
42 3F 3	97.6	2	6512.6	0.0	
43 3F 3	96.1	0	6514.0	0.0	
44 3F 3	98.9	2	6555.9	0.0	
45 3F 3	94.8	0	6570.0	0.0	
46 3F 4	97.3	0	6819.3	0.0	
47 3F 4	95.1	0	6866.8	0.0	
48 3F 4	94.9	2	6896.4	0.0	

TABLE IV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{PrP}_5\text{O}_{14}$ (Cont'd)

FREE ION	PCT PURE	ZMU	THEO. ENERGY	EXP. ENERGY
49 3F 4	99.2	2	6929.0	0.0
50 3F 4	99.3	2	7002.0	0.0
51 3F 4	96.7	0	7029.3	0.0
52 3F 4	98.7	0	7043.4	0.0
53 3F 4	98.4	2	7072.7	0.0
54 3F 4	98.0	0	7091.4	0.0
55 1G 4	99.5	0	9647.3	0.0
56 1G 4	99.8	2	9787.5	0.0
57 1G 4	99.9	0	9790.4	0.0
58 1G 4	99.9	2	9863.4	0.0
59 1G 4	99.9	2	9950.7	0.0
60 1G 4	99.9	0	9965.6	0.0
61 1G 4	99.9	0	10080.2	0.0
62 1G 4	99.8	2	10129.5	0.0
63 1G 4	99.7	0	10157.1	0.0
64 1D 2	100.0	0	16523.0	0.0
65 1D 2	99.9	2	16742.3	0.0
66 1D 2	100.0	0	16748.8	0.0
67 1D 2	99.9	0	16961.4	0.0
68 1D 2	100.0	2	17069.0	0.0

TABLE V. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS,
 B_{km} , for Nd^{3+} in $\text{NdP}_5\text{O}_{14}^a$

ND IN ULTRA PHOS BLATTE ET AL DATA. HOME OVER NITE OF SEPT. 18, 1975.					
FINAL BKM AND CENTRCIDS. 0 = 7.609					
-785.211	= B20	16.203	= B22	-216.583	= B40
290.619	= B60	-242.267	= B62	-274.634	= B62
4I 9/2	182.7			51.669	= B44
4I11/2	2055.4	-620.883	= B44	51.669	= B44
4I13/2	4036.3	18.127	= B66	-175.697	= B66
4I15/2	6083.5				
4F 3/2	11523.6				
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY	
1 4I 9/2	99.6	1	-8.4	0.0*	
2 4I 9/2	99.4	1	86.3	82.0	
3 4I 9/2	99.4	1	195.4	207.0*	
4 4I 9/2	99.6	1	258.3	256.0	
5 4I 9/2	99.7	1	329.3	317.0*	
6 4I11/2	99.4	1	1956.6	1958.0	
7 4I11/2	99.1	1	1981.3	1982.0	
8 4I11/2	99.1	1	2035.1	2044.0*	
9 4I11/2	99.2	1	2075.9	2062.0*	
10 4I11/2	99.3	1	2104.5	2097.0	
11 4I11/2	99.4	1	2166.3	2178.0*	
12 4I13/2	99.5	1	3917.6	3914.0	
13 4I13/2	99.2	1	3945.2	3943.0	
14 4I13/2	99.1	1	3997.8	3995.0	
15 4I13/2	99.6	1	4032.5	4037.0	
16 4I13/2	99.1	1	4078.0	4090.0*	
17 4I13/2	99.5	1	4116.9	4106.0*	
18 4I13/2	99.5	1	4166.7	4171.0	
19 4I15/2	99.4	1	5871.4	5872.0	
20 4I15/2	99.6	1	5910.9	5912.0	
21 4I15/2	99.6	1	6019.1	6011.0*	
22 4I15/2	99.8	1	6065.0	6072.0	
23 4I15/2	99.6	1	6094.4	6081.0*	
24 4I15/2	99.8	1	6207.1	6210.0	
25 4I15/2	99.9	1	6264.0	6274.0*	
26 4I15/2	99.9	1	6287.8	6289.0	
27 4F 3/2	100.0	1	11468.1	11473.0	
28 4F 3/2	100.0	1	11587.4	11583.0	

CENTRCIDS, CRYSTAL = 4043.2 FREE ION = 4043.4

^aThe least-rms deviation between the calculated and experimental energy levels is 7.61 cm^{-1} (M. Blatte, H. G. Danielmeyer, and R. Ulrich, *Appl. Phys.*, 1 (1973), 275).

TABLE VI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
NdP₅O₁₄

NO IN NOP5C14. EXTRAPOLATED BKM FROM COMPATIBLE NO AND EU HOMES. 9/24/75.					
INIT. BKM AND CENTROIDS. Q = -0.000					
-754.900	= 820	153.000	= 822	-158.600	= 840
234.900	= 860	-255.500	= 862	-290.300	= 862
4I 9/2	182.7			183.400	= 864
4I 11/2	2055.4	-470.300	= 344	40.100	= 844
4I 13/2	4036.3	36.500	= 866	-357.300	= 866
4I 15/2	6083.5				
4F 3/2	11523.6				
4F 5/2	12403.0				
2H 9/2 2	12670.0				
4F 7/2	13476.0				
4S 3/2	13583.0				
4F 9/2	14760.0				
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY	
1 4I 9/2	99.5	1	-4.6	0.0	
2 4I 9/2	99.6	1	73.8	0.0	
3 4I 9/2	99.5	1	201.0	0.0	
4 4I 9/2	99.4	1	256.5	0.0	
5 4I 9/2	99.7	1	326.6	0.0	
6 4I 11/2	99.5	1	1960.3	0.0	
7 4I 11/2	99.2	1	1973.2	0.0	
8 4I 11/2	99.1	1	2031.5	0.0	
9 4I 11/2	99.0	1	2083.7	0.0	
10 4I 11/2	99.3	1	2100.7	0.0	
11 4I 11/2	99.5	1	2161.8	0.0	
12 4I 13/2	99.4	1	3920.8	0.0	
13 4I 13/2	99.4	1	3942.8	0.0	
14 4I 13/2	99.2	1	3990.3	0.0	
15 4I 13/2	99.3	1	4022.3	0.0	
16 4I 13/2	99.1	1	4086.1	0.0	
17 4I 13/2	99.4	1	4112.0	0.0	
18 4I 13/2	99.6	1	4163.5	0.0	
19 4I 15/2	99.4	1	5865.5	0.0	
20 4I 15/2	99.5	1	5921.0	0.0	
21 4I 15/2	99.8	1	6016.7	0.0	
22 4I 15/2	99.7	1	6048.4	0.0	
23 4I 15/2	99.5	1	6083.3	0.0	
24 4I 15/2	99.8	1	6212.9	0.0	
25 4I 15/2	99.9	1	6255.0	0.0	
26 4I 15/2	99.9	1	6293.3	0.0	
27 4F 3/2	98.6	1	11451.7	0.0	
28 4F 3/2	98.9	1	11576.6	0.0	
29 4F 5/2	97.3	1	12336.0	0.0	
30 4F 5/2	94.9	1	12399.8	0.0	
31 4F 5/2	96.4	1	12462.0	0.0	
32 2H 9/2 2	98.3	1	12577.6	0.0	
33 2H 9/2 2	96.8	1	12603.0	0.0	
34 2H 9/2 2	98.5	1	12678.1	0.0	
35 2H 9/2 2	98.5	1	12754.5	0.0	
36 2H 9/2 2	98.9	1	12755.3	0.0	
37 4F 7/2	99.0	1	13370.7	0.0	
38 4F 7/2	98.6	1	13475.9	0.0	
39 4F 7/2	98.7	1	13493.9	0.0	
40 4S 3/2	85.5	1	13579.3	0.0	
41 4F 7/2	64.9	1	13589.5	0.0	
42 4S 3/2	79.5	1	13593.1	0.0	

TABLE VI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{NdP}_5\text{O}_{14}$ (Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
43 4F 9/2	99.6	1	14655.2	0.C
44 4F 9/2	99.6	1	14711.5	0.C
45 4F 9/2	99.3	1	14793.8	0.C
46 4F 9/2	99.8	1	14837.6	0.C
47 4F 9/2	99.8	1	14850.0	0.C

TABLE VII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
PmP₅O₁₄

PN IN PMP5O14. EXTRAPOLATED BKM FROM COMPATIBLE ND AND EU MODELS. 9/24/75.						
INIT.	BKM AND CENTRCIDS.	Q = -0.000				
	-729.300 = B20	147.800 = B22	-152.800 = B40	-307.400 = B42	698.300 = B42	
	229.500 = B60	235.800 = B62	-295.300 = B62	207.700 = B64	-261.200 = B64	
S1 4	233.0					
S1 5	1731.0	-65.700 = B44	456.600 = B44			
S1 6	3306.0	-138.800 = B66	-322.400 = B66			
S1 7	4953.0					
S1 8	6716.0					
SF 1	12298.0					
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY		
1 51 4	99.7	0	115.9	0.0		
2 51 4	99.7	2	142.6	0.0		
3 51 4	99.7	0	142.9	0.0		
4 51 4	99.4	2	153.7	0.0		
5 51 4	99.2	0	169.5	0.0		
6 51 4	98.9	2	215.2	0.0		
7 51 4	99.5	0	286.9	0.0		
8 51 4	98.5	0	355.3	0.0		
9 51 4	98.9	2	399.1	0.0		
10 51 5	99.8	2	1620.5	0.0		
11 51 5	99.6	2	1633.3	0.0		
12 51 5	98.9	0	1697.4	0.0		
13 51 5	99.3	0	1700.9	0.0		
14 51 5	99.1	2	1710.2	0.0		
15 51 5	99.3	0	1721.2	0.0		
16 51 5	98.5	2	1738.2	0.0		
17 51 5	99.0	0	1770.2	0.0		
18 51 5	98.2	2	1792.6	0.0		
19 51 5	99.6	2	1809.6	0.0		
20 51 5	98.2	0	1827.0	0.0		
21 51 6	99.7	0	3200.2	0.0		
22 51 6	99.8	0	3201.9	0.0		
23 51 6	99.4	2	3258.2	0.0		
24 51 6	99.5	2	3270.5	0.0		
25 51 6	98.9	0	3281.8	0.0		
26 51 6	99.1	2	3287.1	0.0		
27 51 6	98.7	0	3305.2	0.0		
28 51 6	98.8	2	3319.5	0.0		
29 51 6	99.1	0	3326.2	0.0		
30 51 6	99.1	0	3364.8	0.0		
31 51 6	98.6	2	3366.5	0.0		
32 51 6	99.4	0	3388.6	0.0		
33 51 6	99.4	2	3391.1	0.0		
34 51 7	99.7	2	4455.9	0.0		
35 51 7	99.8	2	4854.4	0.0		
36 51 7	99.3	0	4882.5	0.0		
37 51 7	99.8	0	4885.6	0.0		
38 51 7	99.0	2	4888.5	0.0		
39 51 7	99.2	0	4891.8	0.0		
40 51 7	99.4	2	4936.7	0.0		
41 51 7	99.4	2	4939.7	0.0		
42 51 7	98.9	0	4981.9	0.0		
43 51 7	98.9	0	4992.2	0.0		
44 51 7	99.1	2	5017.8	0.0		
45 51 7	99.0	2	5031.3	0.0		
46 51 7	99.1	0	5039.3	0.0		
47 51 7	99.1	0	5051.1	0.0		
48 51 7	99.1	2	5052.1	0.0		
49 51 8	100.0	0	6547.6	0.0		
50 51 8	100.0	2	6548.1	0.0		
51 51 8	99.9	0	6586.4	0.0		
52 51 8	99.9	2	6588.2	0.0		
53 51 8	99.8	0	6591.1	0.0		
54 51 8	99.8	2	6595.4	0.0		
55 51 8	99.8	0	6670.7	0.0		
56 51 8	99.8	0	6682.3	0.0		
57 51 8	99.7	2	6694.4	0.0		
58 51 8	99.5	2	6731.2	0.0		
59 51 8	99.5	0	6751.5	0.0		
60 51 8	99.7	2	6814.8	0.0		

TABLE VII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{PmP}_5\text{O}_{14}$

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
61 5I 8	99.6	0	6422.5	0.0
62 5I 8	99.6	0	6491.5	0.0
63 5I 8	99.6	2	6494.5	0.0
64 5I 8	99.0	2	6444.2	0.0
65 5I 8	99.0	0	6444.8	0.0
66 5F 1	100.0	0	12241.3	0.0
67 5F 1	100.0	2	12317.9	0.0
68 5F 1	100.0	2	12346.4	0.0

TABLE VIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR SmP₅O₁₄

SM IN SMP5014. EXTERPOLATED BKM FROM COMPATIBLE NO AND EU MODELS. 9/24/75.					
INIT. 8KM AND CENTRCIOS. Q = -0.000					
-702.700	= B20	142.400	= B22	-146.700	= B40
224.100	= B60	323.900	= B62	176.400	= B62
6H 5/2	134.0			363.800	= B42
6H 7/2	1183.0	415.100	= B44	160.000	= B44
6H 9/2	2398.0	-271.500	= B66	-208.900	= B66
6H11/2	3737.0				
6H13/2	5098.0				
6F 1/2	6355.0				
6H15/2	6550.0				
6F 3/2	6700.0				
6F 5/2	7116.0				
6F 7/2	7995.0				
6F 9/2	9147.0				
FREE ION	PCT	PURE	2MU	THEO. ENERGY	EXP. ENERGY
1 6H 5/2	98.6	1		-52.5	0.C
2 6H 5/2	98.6	1		136.7	0.C
3 6H 5/2	98.4	1		239.4	0.C
4 6H 7/2	98.6	1		1021.4	0.C
5 6H 7/2	98.1	1		1132.7	0.C
6 6H 7/2	97.4	1		1219.0	0.C
7 6H 7/2	98.5	1		1316.3	0.C
8 6H 9/2	98.6	1		2252.6	0.C
9 6H 9/2	98.2	1		2305.3	0.C
10 6H 9/2	98.4	1		2403.2	0.O
11 6H 9/2	98.2	1		2458.7	0.C
12 6H 9/2	98.9	1		2524.6	0.C
13 6H11/2	98.9	1		3566.7	0.C
14 6H11/2	98.1	1		3634.3	0.C
15 6H11/2	98.4	1		3713.8	0.C
16 6H11/2	98.2	1		3766.1	0.O
17 6H11/2	98.6	1		3820.0	0.C
18 6H11/2	98.7	1		3861.0	0.O
19 6H13/2	99.0	1		4882.3	0.C
20 6H13/2	98.3	1		4977.6	0.C
21 6H13/2	97.7	1		5075.7	0.O
22 6H13/2	98.4	1		5111.6	0.C
23 6H13/2	97.8	1		5155.5	0.C
24 6H13/2	98.6	1		5191.0	0.C
25 6H13/2	98.2	1		5224.5	0.C
26 6H15/2	98.4	1		6267.1	0.C
27 6F 1/2	95.5	1		6364.0	0.C
28 6H15/2	96.2	1		6383.3	0.C
29 6H15/2	98.2	1		6447.3	0.C
30 6H15/2	97.4	1		6516.8	0.C
31 6H15/2	97.8	1		6574.9	0.O
32 6H15/2	93.4	1		6664.5	0.C
33 6F 3/2	91.4	1		6699.8	0.C
34 6F 3/2	75.5	1		6726.1	0.C
35 6H15/2	89.5	1		6741.6	0.C
36 6H15/2	85.1	1		6790.2	0.C
37 6F 5/2	97.2	1		7114.2	0.C
38 6F 5/2	94.4	1		7153.8	0.C
39 6F 5/2	96.7	1		7166.9	0.C

TABLE VIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
SmP₅O₁₄

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
40 6F 7/2	98.5	1	7967.4	0.0
41 6F 7/2	98.7	1	8009.0	0.0
42 6F 7/2	99.0	1	8026.5	0.0
43 6F 7/2	98.5	1	8063.8	0.0
44 6F 9/2	99.5	1	9107.9	0.0
45 6F 9/2	99.5	1	9134.2	0.0
46 6F 9/2	99.4	1	9179.4	0.0
47 6F 9/2	99.1	1	9194.1	0.0
48 6F 9/2	99.3	1	9219.2	0.0

TABLE IX. ENERGY LEVELS AND PHENOMENOLOGICAL B_{km} for Eu^{3+} IN $\text{EuP}_5\text{O}_{14}^{\text{a}}$

EU IN P5O14. NEW ASSIGNMENTS BASED ON SCALED BKM FROM ND HOMF. 9/22975.					
FINAL BKM AND CENTROIDS. Q = 13.182					
-585.724	= B20	-212.651	= B22	-83.130	= B40
131.526	= B60	117.952	= B62	-387.768	= B62
7F 0	31.5			80.858	= B64
7F 1	405.1	111.358	= B44	-183.577	= B44
7F 2	1071.3	457.164	= B66	2.900	= B66
7F 3	1935.4				
7F 4	2900.5				
7F 5	3919.3				
7F 6	5003.1				
FREE ION	PCT	PURE	ZMU	THEO. ENERGY	EXP. ENERGY
1	7F 0	97.9	0	0.0	0.0
2	7F 1	99.2	0	272.1	271.0
3	7F 1	98.1	2	388.8	392.0
4	7F 1	97.4	2	476.3	474.0
5	7F 2	98.9	0	951.8	937.0*
6	7F 2	97.0	2	971.3	960.0
7	7F 2	97.5	2	1061.3	1070.0
8	7F 2	95.0	0	1091.7	1097.0
9	7F 2	95.8	0	1168.2	1180.0
10	7F 3	98.5	2	1854.8	1869.0*
11	7F 3	97.9	0	1886.2	1876.0
12	7F 3	94.6	2	1902.1	1890.0
13	7F 3	93.4	0	1911.9	1919.0
14	7F 3	97.0	2	1960.6	1928.0*
15	7F 3	94.7	0	1970.6	1982.0
16	7F 3	97.6	2	1991.2	2012.0*
17	7F 4	97.3	0	2742.2	2741.0
18	7F 4	95.5	2	2783.9	2794.0
19	7F 4	97.9	0	2833.6	2811.0*
20	7F 4	95.9	2	2837.4	2844.0
21	7F 4	96.5	0	2877.9	2869.0
22	7F 4	95.4	0	2969.2	2973.0
23	7F 4	97.4	2	2974.7	2979.0
24	7F 4	97.8	2	3002.5	3007.0
25	7F 4	97.8	0	3037.8	3040.0
26	7F 5	98.7	2	3754.2	3748.0
27	7F 5	98.1	2	3776.9	3774.0
28	7F 5	96.6	0	3839.7	3864.0*
29	7F 5	96.4	0	3900.7	3893.0
30	7F 5	94.8	0	3911.8	3907.0
31	7F 5	94.3	2	3919.3	3918.0
32	7F 5	97.3	2	3946.5	3929.0*
33	7F 5	98.5	2	3983.1	3984.0
34	7F 5	96.3	0	4006.2	4018.0
35	7F 5	97.4	0	4045.8	4049.0
36	7F 5	97.9	2	4059.4	4061.0
37	7F 6	99.2	0	4811.7	4798.0*
38	7F 6	99.1	0	4812.7	4811.0
39	7F 6	98.6	2	4907.4	4928.0*
40	7F 6	98.4	2	4913.4	4952.0*
41	7F 6	99.1	0	4966.4	4962.0
42	7F 6	99.2	2	4972.2	4980.0

^aThe least-rms deviation between the calculated and experimental energy levels is 10.43 cm^{-1} (C. Brecher, J. Chem. Phys., 61 (1974), 2297).

TABLE IX. ENERGY LEVELS AND PHENOMENOLOGICAL B_{km} FOR Eu^{3+} IN $\text{EuP}_5\text{O}_{14}^{\text{a}}$
(Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
43 7F 6	97.8	0	5024.2	4993.C*
44 7F 6	96.7	0	5047.6	5042.C
45 7F 6	97.0	2	5064.1	5057.C
46 7F 6	97.3	0	5145.6	5138.C
47 7F 6	97.5	2	5148.4	5160.C
48 7F 6	99.4	2	5266.6	5250.C*
49 7F 6	99.4	0	5266.9	5277.C

^aThe least-rms deviation between the calculated and experimental energy levels is 10.43 cm^{-1} (C. Brecher, J. Chem. Phys., 61 (1974), 2297).

TABLE X. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
EuP₅O₁₄

EU IN EUP5O14. EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.					
INIT. BKM AND CENTRCDS. Q = -0.000					
-675.000	= B20	136.800	= B22	-140.400	= B40
218.400	= B60	-114.300	= B62	340.900	= B62
7F 0	96.0			236.100	= B44
7F 1	473.0			-330.400	= B66
7F 2	1175.0				
7F 3	1998.0				
7F 4	3000.0				
7F 5	4073.0				
7F 6	5094.0				
SD 0 3	17220.0				
SD 1 3	18960.0				
SD 2 3	21422.0				
SD 3 3	24653.0				
FREE ION	PCT	PURE	2MU	THEO. ENERGY	EXP. ENERGY
1 7F 0		97.6	0	61.1	0.0
2 7F 1	39.2	0		321.6	0.0
3 7F 1	97.6	2		478.7	0.0
4 7F 1	96.9	2		531.7	0.0
5 7F 2	96.7	2		1062.3	0.0
6 7F 2	98.1	0		1065.2	0.0
7 7F 2	96.9	2		1159.2	0.0
8 7F 2	93.5	0		1179.9	0.0
9 7F 2	95.9	0		1285.1	0.0
10 7F 3	98.2	2		1918.5	0.0
11 7F 3	97.3	0		1955.4	0.0
12 7F 3	95.1	2		1967.1	0.0
13 7F 3	92.2	0		1987.1	0.0
14 7F 3	96.8	2		2019.3	0.0
15 7F 3	94.3	0		2034.3	0.0
16 7F 3	96.7	2		2044.6	0.0
17 7F 4	97.4	0		2835.2	0.0
18 7F 4	95.3	2		2885.7	0.0
19 7F 4	97.4	0		2916.0	0.0
20 7F 4	95.7	2		2955.9	0.0
21 7F 4	96.2	0		3000.6	0.0
22 7F 4	96.2	0		3066.5	0.0
23 7F 4	97.5	2		3073.1	0.0
24 7F 4	97.7	2		3082.5	0.0
25 7F 4	97.5	0		3143.2	0.0
26 7F 5	98.4	2		3906.5	0.0
27 7F 5	97.9	2		3922.0	0.0
28 7F 5	94.9	0		4016.5	0.0
29 7F 5	96.6	0		4027.4	0.0
30 7F 5	93.2	2		4030.4	0.0
31 7F 5	94.5	0		4045.4	0.0
32 7F 5	97.9	2		4104.5	0.0
33 7F 5	97.7	2		4129.9	0.0
34 7F 5	96.5	0		4178.1	0.0
35 7F 5	97.5	0		4212.7	0.0
36 7F 5	98.3	2		4236.4	0.0
37 7F 6	99.2	0		4877.4	0.0
38 7F 6	99.0	0		4879.5	0.0
39 7F 6	98.2	2		4981.0	0.0
40 7F 6	98.0	2		4986.2	0.0
41 7F 6	98.2	0		5077.6	0.0
42 7F 6	98.2	2		5092.3	0.0
43 7F 6	96.3	0		5126.4	0.0

TABLE X. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
EuP₅O₁₄ (Cont'd)

FREE ION	PCT	PURE	2MU	THEO. ENERGY	EXP. ENERGY
44 7F 6		96.5	0	5156.7	0.0
45 7F 6		96.6	2	5190.9	0.C
46 7F 6		98.0	2	5244.8	0.C
47 7F 6		98.0	0	5244.4	0.C
48 7F 6		99.4	2	5349.1	0.C
49 7F 6		99.4	0	5349.2	0.C
50 5D 0	3	100.0	0	17219.4	0.C
51 5D 1	3	100.0	0	18920.9	0.C
52 5D 1	3	100.0	2	18968.9	0.C
53 5D 1	3	100.0	2	18988.6	0.C
54 5D 2	3	100.0	2	21401.2	0.C
55 5D 2	3	100.0	0	21404.2	0.C
56 5D 2	3	100.0	0	21418.5	0.C
57 5D 2	3	100.0	2	21439.8	0.C
58 5D 2	3	100.0	0	21445.2	0.C
59 5D 3	3	100.0	2	24618.2	0.C
60 5D 3	3	100.0	2	24629.1	0.C
61 5D 3	3	100.0	0	24651.3	0.C
62 5D 3	3	100.0	0	24651.9	0.0
63 5D 3	3	100.0	2	24655.4	0.C
64 5D 3	3	100.0	0	24683.7	0.C
65 5D 3	3	100.0	2	24684.9	0.C

TABLE XI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR GdP₅O₁₄

GD IN GdP ₅ O ₁₄ . EXTRAPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.						
INIT.	BKM AND CENTRCIDS.	Q = -0.00J				
-646.200	= B20	131.000 = B22	-133.700 = B4C	456.700 = B42	-487.100 = B42	
212.700	= B60	-346.300 = B62	-51.700 = B62	257.700 = B64	-170.700 = B64	
BS 7/2	0.0					
6P 7/2	32210.0	-276.800 = B44	-296.300 = B44			
6P 5/2	32753.0	-304.200 = B66	114.900 = B66			
6P 3/2	33289.0					
6I 7/2	35865.0					
6I 9/2	36217.0					
6I 17/2	36448.0					
6I 11/2	36516.0					
6I 13/2	36700.0					
6I 15/2	36711.0					
FREE ION	PCT PURE	ZMU	THEO. ENERGY	EXP. ENERGY		
1 BS 7/2	100.0	1	-0.4	0.C		
2 BS 7/2	100.0	1	-0.2	0.C		
3 BS 7/2	100.0	1	0.0	0.C		
4 BS 7/2	100.0	1	0.3	0.C		
5 6P 7/2	99.8	1	32137.7	0.C		
6 6P 7/2	99.7	1	32177.6	0.C		
7 6P 7/2	99.6	1	32213.5	0.C		
8 6P 7/2	99.8	1	32272.0	0.C		
9 6P 5/2	99.6	1	32713.0	0.C		
10 6P 5/2	98.6	1	32733.9	0.C		
11 6P 5/2	99.4	1	32777.5	0.C		
12 6P 3/2	98.9	1	33261.1	0.C		
13 6P 3/2	99.4	1	33299.3	0.C		
14 6I 7/2	100.0	1	35842.9	0.C		
15 6I 7/2	99.9	1	35863.6	0.C		
16 6I 7/2	99.8	1	35877.7	0.C		
17 6I 7/2	99.9	1	35886.9	0.C		
18 6I 9/2	99.9	1	36188.9	0.C		
19 6I 9/2	99.9	1	36205.0	0.C		
20 6I 9/2	99.7	1	36225.4	0.C		
21 6I 9/2	99.7	1	36231.3	0.C		
22 6I 9/2	99.8	1	36245.3	0.C		
23 6I 17/2	98.6	1	36445.6	0.C		
24 6I 17/2	98.7	1	36445.7	0.C		
25 6I 17/2	99.3	1	36446.1	0.C		
26 6I 17/2	99.2	1	36446.2	0.C		
27 6I 17/2	99.0	1	36447.4	0.C		
28 6I 17/2	99.1	1	36448.3	0.C		
29 6I 17/2	98.2	1	36450.3	0.C		
30 6I 17/2	99.0	1	36453.5	0.C		
31 6I 17/2	99.1	1	36455.5	0.C		
32 6I 11/2	97.5	1	36485.5	0.0		
33 6I 11/2	97.9	1	36502.1	0.0		
34 6I 11/2	98.9	1	36511.1	0.C		
35 6I 11/2	98.6	1	36527.6	0.C		
36 6I 11/2	98.9	1	36535.8	0.0		
37 6I 11/2	98.9	1	36546.9	0.0		
38 6I 13/2	88.3	1	36666.0	0.C		
39 6I 13/2	88.6	1	36681.9	0.C		
40 6I 13/2	52.3	1	36686.4	0.C		
41 6I 13/2	52.0	1	36690.5	0.C		
42 6I 15/2	57.0	1	36693.6	0.C		
43 6I 15/2	82.6	1	36701.3	0.C		
44 6I 15/2	65.9	1	36706.8	0.C		

TABLE XI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
GdP₅O₁₄ (Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
45 6I15/2	74.3	1	36710.6	0.0
46 6I15/2	54.3	1	36713.1	0.0
47 6I13/2	65.8	1	36717.5	0.0
48 6I13/2	55.9	1	36723.0	0.0
49 6I15/2	50.6	1	36726.3	0.0
50 6I15/2	79.3	1	36731.2	0.0
51 6I15/2	80.9	1	36741.8	0.0
52 6I15/2	57.0	1	36743.5	0.0

TABLE XII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 TbP_5O_{14}

TB IN TBP5C14. EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.					
INIT. BKM AND CENTRC10S. Q = -0.000					
-616.000	= B20	124.900	= B22	-126.700	= B40
206.700	= B60	-9.200	= B62	-340.200	= B62
7F 6	310.0			266.500	= B64
7F 5	2347.0	-332.400	= 344	192.400	= B44
7F 4	3580.0	-203.900	= B66	241.400	= B66
7F 3	4573.0				
7F 2	5155.0				
7F 1	5432.0				
7F 0	5766.0				
SD 4 3	20569.0				
SD 3 3	26357.0				
FREE ION	PCT PURE	ZMU	THEO. ENERGY	EXP. ENERGY	
1 7F 6	99.6	2	88.8	0.C	
2 7F 6	99.6	0	89.4	0.C	
3 7F 6	99.3	0	170.7	0.C	
4 7F 6	99.1	2	192.7	0.C	
5 7F 6	99.3	2	215.9	0.C	
6 7F 6	99.6	0	265.6	0.C	
7 7F 6	99.8	2	289.1	0.C	
8 7F 6	99.0	0	311.1	0.C	
9 7F 6	99.3	0	313.4	0.C	
10 7F 6	99.8	2	441.6	0.C	
11 7F 6	99.8	2	447.8	0.C	
12 7F 6	99.8	0	515.8	0.C	
13 7F 6	99.8	0	518.4	0.C	
14 7F 5	98.7	2	2196.0	0.C	
15 7F 5	98.6	0	2213.3	0.C	
16 7F 5	97.9	0	2249.5	0.C	
17 7F 5	98.9	2	2294.8	0.C	
18 7F 5	96.7	0	2298.9	0.C	
19 7F 5	98.6	2	2322.9	0.C	
20 7F 5	99.2	0	2381.1	0.C	
21 7F 5	98.7	2	2387.9	0.C	
22 7F 5	98.7	0	2444.4	0.C	
23 7F 5	99.1	2	2465.0	0.C	
24 7F 5	99.4	2	2489.1	0.C	
25 7F 4	97.8	0	3404.3	0.C	
26 7F 4	97.6	2	3495.5	0.C	
27 7F 4	95.2	0	3543.6	0.C	
28 7F 4	97.7	2	3547.1	0.C	
29 7F 4	97.3	2	3595.3	0.C	
30 7F 4	99.3	0	3603.7	0.C	
31 7F 4	99.6	0	3648.4	0.C	
32 7F 4	97.1	2	3658.3	0.C	
33 7F 4	98.0	0	3720.2	0.C	
34 7F 3	97.0	2	4522.0	0.C	
35 7F 3	91.5	0	4528.0	0.C	
36 7F 3	95.7	2	4547.8	0.C	
37 7F 3	96.4	0	4578.2	0.C	
38 7F 3	92.5	0	4592.2	0.C	
39 7F 3	95.2	2	4593.5	0.C	
40 7F 3	97.7	2	4647.0	0.C	
41 7F 2	93.4	0	5067.6	0.C	
42 7F 2	91.5	2	5137.1	0.C	
43 7F 2	91.2	0	5177.6	0.C	
44 7F 2	94.9	0	5217.1	0.C	
45 7F 2	80.8	2	5250.1	0.C	
46 7F 1	80.4	2	5393.4	0.C	
47 7F 1	89.9	2	5451.8	0.C	
48 7F 1	98.0	0	5579.1	0.C	

TABLE XII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 TbP_5O_{14} (Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
49 7F 0		94.0	0	5812.3
50 5D 4	3	100.0	0	20517.2
51 5D 4	3	100.0	2	20524.2
52 5D 4	3	100.0	0	20546.1
53 5D 4	3	100.0	2	20549.3
54 5D 4	3	100.0	0	20563.2
55 5D 4	3	100.0	2	20581.8
56 5D 4	3	100.0	2	20587.1
57 5D 4	3	100.0	0	20623.3
58 5D 4	3	100.0	0	20626.8
59 5D 3	3	100.0	2	26347.7
60 5D 3	3	100.0	0	26348.7
61 5D 3	3	100.0	0	26351.2
62 5D 3	3	100.0	2	26354.4
63 5D 3	3	100.0	2	26362.5
64 5D 3	3	100.0	2	26368.4
65 5D 3	3	100.0	0	26368.6

TABLE XIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
DyP₅O₁₄

DY IN DYP5C14. EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.					
INIT. BKM AND CENTRCIOS. Q = -0.CCO					
-584.300	= 820	118.500	= 822	-115.300	= 840
200.600	= 860	323.500	= 862	-66.400	= 862
6H15/2	262.0			271.300	= 864
6H13/2	3710.0	106.800	= 344	345.700	= 344
6H11/2	6028.0	-58.800	= 866	301.100	= 866
6F11/2	7830.0				
6H 9/2	7879.0				
6F 9/2	9188.0				
6H 7/2	9243.0				
6H 5/2	10340.0				
6F 7/2	11071.0				
6F 5/2	12462.0				
FREE ION PCT PURE 2MU THEO. ENERGY EXP. ENERGY					
1 6H15/2	100.0	1	32.7	0.C	
2 6H15/2	99.9	1	137.8	0.C	
3 6H15/2	99.9	1	176.0	0.C	
4 6H15/2	99.9	1	230.2	0.C	
5 6H15/2	99.9	1	262.2	0.C	
6 6H15/2	99.9	1	311.5	0.C	
7 6H15/2	99.9	1	378.4	0.O	
8 6H15/2	99.9	1	508.0	0.C	
9 6H13/2	99.9	1	3554.6	0.C	
10 6H13/2	99.7	1	3622.6	0.C	
11 6H13/2	99.6	1	3672.3	0.C	
12 6H13/2	99.8	1	3686.2	0.C	
13 6H13/2	99.8	1	3725.9	0.C	
14 6H13/2	99.6	1	3798.0	0.C	
15 6H13/2	99.7	1	3861.9	0.C	
16 6H11/2	99.4	1	5923.2	0.C	
17 6H11/2	99.2	1	5957.9	0.C	
18 6H11/2	99.2	1	5971.9	0.C	
19 6H11/2	99.4	1	6015.8	0.C	
20 6H11/2	99.2	1	6093.6	0.C	
21 6H11/2	99.5	1	6156.8	0.C	
22 6F11/2	59.4	1	7704.5	0.C	
23 6F11/2	49.7	1	7734.5	0.C	
24 6F11/2	56.7	1	7767.0	0.C	
25 6F11/2	52.8	1	7783.4	0.C	
26 6F11/2	78.2	1	7810.5	0.C	
27 6F11/2	73.1	1	7833.0	0.C	
28 6F11/2	67.6	1	7872.3	0.C	
29 6H 9/2	64.4	1	7900.9	0.C	
30 6F11/2	65.1	1	7944.7	0.C	
31 6H 9/2	70.7	1	7977.5	0.C	
32 6H 9/2	66.7	1	8047.3	0.C	
33 6F 9/2	53.6	1	9058.6	0.C	
34 6H 7/2	58.9	1	9107.7	0.C	
35 6F 9/2	62.3	1	9144.5	0.C	
36 6F 9/2	87.3	1	9182.5	0.C	
37 6F 9/2	87.9	1	9211.1	0.C	
38 6F 9/2	78.8	1	9235.3	0.C	
39 6H 7/2	63.5	1	9281.6	0.O	
40 6H 7/2	61.9	1	9328.0	0.C	
41 6H 7/2	83.9	1	9392.1	0.C	

TABLE XIII. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{DyP}_5\text{O}_{14}$ (Cont'd)

FREE ION	PCT. PURE	2MU	THEO. ENERGY	EXP. ENERGY
42 6H 5/2	96.9	1	10228.6	0.C
43 6H 5/2	97.7	1	10332.4	0.C
44 6H 5/2	95.3	1	10464.7	0.C
45 6F 7/2	97.6	1	11057.1	0.0
46 6F 7/2	99.1	1	11085.1	0.C
47 6F 7/2	97.5	1	11102.0	0.0
48 6F 7/2	98.7	1	11122.1	0.C
49 6F 5/2	99.6	1	12447.9	0.C
50 6F 5/2	99.8	1	12482.5	0.C
51 6F 5/2	99.6	1	12495.9	0.C

TABLE XIV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
HoP₅O₁₄

HO IN HOP5C14. EXTRPOLATED BKM FROM COMPATIBLE NO AND EU HOMES. 9/24/75.					
INIT. PKM AND CENTRICALS. Q = -0.000	-550.800 = B20	111.700 = B22	-111.400 = B40	-493.800 = B42	256.500 = B44
	-194.300 = B60	117.900 = B62	297.400 = B62	272.200 = B64	-75.600 = B64
51 8	169.6				
51 7	5219.5	337.000 = B44	-25.000 = B44		
51 6	8717.6	.92.300 = B66	282.500 = B66		
51 5	11274.7				
51 4	13333.4				
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY	
1 51 8	100.0	0	17.0	0.0	
2 51 8	100.0	2	18.9	0.0	
3 51 8	100.0	2	31.4	0.0	
4 51 8	100.0	0	40.7	0.0	
5 51 8	100.0	0	69.1	0.0	
6 51 8	100.0	2	102.6	0.0	
7 51 8	100.0	0	138.4	0.0	
8 51 8	100.0	2	167.3	0.0	
9 51 8	100.0	0	17C.2	0.0	
10 51 8	100.0	2	201.6	0.0	
11 51 8	100.0	0	226.8	0.0	
12 51 8	100.0	0	246.9	0.0	
13 51 8	100.0	2	247.3	0.0	
14 51 8	100.0	2	275.8	0.0	
15 51 8	100.0	2	286.3	0.0	
16 51 8	100.0	0	303.3	0.0	
17 51 8	100.0	0	306.6	0.0	
18 51 7	100.0	0	513b.6	0.0	
19 51 7	100.0	2	513H.7	0.0	
20 51 7	100.0	2	5183.1	0.0	
21 51 7	99.9	0	5183.3	0.0	
22 51 7	99.9	2	5197.2	0.0	
23 51 7	99.9	0	5197.7	0.0	
24 51 7	99.9	2	5205.0	0.0	
25 51 7	100.0	0	5205.0	0.0	
26 51 7	99.9	2	5228.3	0.0	
27 51 7	99.9	0	5232.5	0.0	
28 51 7	99.9	2	5240.4	0.0	
29 51 7	99.9	0	5268.2	0.0	
30 51 7	99.9	0	5269.7	0.0	
31 51 7	99.9	2	5296.3	0.0	
32 51 7	100.0	2	5296.4	0.0	
33 51 6	99.9	2	8639.8	0.0	
34 51 6	99.9	0	8640.7	0.0	
35 51 6	99.9	0	8689.3	0.0	
36 51 6	99.9	2	8692.5	0.0	
37 51 6	99.9	2	8705.5	0.0	
38 51 6	99.8	0	870H.3	0.0	
39 51 6	99.8	0	8715.4	0.0	
40 51 6	99.8	2	8720.4	0.0	
41 51 6	99.9	0	8735.0	0.0	
42 51 6	99.8	2	8745.9	0.0	
43 51 6	99.8	2	8751.4	0.0	
44 51 6	99.9	0	8788.5	0.0	
45 51 6	99.9	0	879C.0	0.0	
46 51 5	99.7	0	11209.3	0.0	
47 51 5	99.9	2	11211.4	0.0	
48 51 5	99.8	0	11254.2	0.0	
49 51 5	99.6	2	11256.7	0.0	
50 51 5	99.8	2	11265.3	0.0	
51 51 5	99.7	0	11269.2	0.0	
52 51 5	99.9	2	11285.4	0.0	
53 51 5	99.5	0	11288.4	0.0	
54 51 5	99.8	0	11305.7	0.0	

TABLE XIV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{HoP}_5\text{O}_{14}$ (Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
55 5I 5	99.5	2	11332.2	0.C
56 5I 5	99.0	2	11341.1	0.C
57 5I 4	99.8	0	13244.2	0.C
58 5I 4	99.7	2	13244.6	0.C
59 5I 4	99.8	0	13285.0	0.C
60 5I 4	99.7	0	13298.7	0.C
61 5I 4	99.5	2	13328.1	0.C
62 5I 4	99.8	2	13336.7	0.C
63 5I 4	99.9	2	13426.9	0.C
64 5I 4	99.8	0	13427.6	0.C
65 5I 4	100.0	0	13462.8	0.C

TABLE XV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR ErP₅O₁₄

ER IN ERP5O14. EXTERPOLATED BKM FROM COMPATIBLE ND AND EU HOMES. 9/24/75.					
INIT. BKM AND CENTRICALS. Q = -0.000					
-515.000	= B20	104.400	= B22	-102.900	= B40
187.800	= B60	-263.100	= B62	162.300	= B62
4I15/2	263.0			269.300	= B64
4I13/2	6736.0	47.200	= B44	-308.500	= B44
4I11/2	10346.0	210.800	= B66	195.100	= B66
4I 9/2	12560.0				
4F 9/2	15365.0				
4S 3/2	18444.0				
2H11/2 2	19190.0				
4F 7/2	20582.0				
4F 5/2	22230.0				
4F 3/2	22561.0				
FREE ION PCT PURE 2MU THEO. ENERGY EXP. ENERGY					
1 4I15/2	100.0	1	87.5	0.C	
2 4I15/2	100.0	1	119.0	0.C	
3 4I15/2	100.0	1	199.3	0.C	
4 4I15/2	100.0	1	251.7	0.C	
5 4I15/2	100.0	1	306.1	0.C	
6 4I15/2	100.0	1	337.9	0.C	
7 4I15/2	100.0	1	369.6	0.C	
8 4I15/2	100.0	1	413.5	0.C	
9 4I13/2	100.0	1	6632.6	0.C	
10 4I13/2	99.9	1	6668.6	0.C	
11 4I13/2	99.9	1	6717.9	0.C	
12 4I13/2	99.9	1	6733.3	0.C	
13 4I13/2	100.0	1	6782.0	0.C	
14 4I13/2	100.0	1	6795.0	0.C	
15 4I13/2	100.0	1	6804.2	0.C	
16 4I11/2	99.9	1	10289.2	0.C	
17 4I11/2	99.9	1	10316.4	0.C	
18 4I11/2	99.9	1	10340.7	0.C	
19 4I11/2	99.9	1	10363.9	0.C	
20 4I11/2	99.9	1	10372.1	0.C	
21 4I11/2	100.0	1	10389.6	0.C	
22 4I 9/2	99.9	1	12458.6	0.C	
23 4I 9/2	99.9	1	12477.0	0.C	
24 4I 9/2	100.0	1	12585.7	0.C	
25 4I 9/2	100.0	1	12612.5	0.C	
26 4I 9/2	100.0	1	12661.7	0.C	
27 4F 9/2	99.9	1	15289.2	0.C	
28 4F 9/2	100.0	1	15344.6	0.C	
29 4F 9/2	100.0	1	15362.0	0.C	
30 4F 9/2	99.9	1	15407.1	0.C	
31 4F 9/2	99.9	1	15428.3	0.C	
32 4S 3/2	99.3	1	18409.0	0.C	
33 4S 3/2	98.9	1	18468.4	0.C	
34 2H11/2 2	99.7	1	19144.8	0.C	
35 2H11/2 2	99.3	1	19164.0	0.C	
36 2H11/2 2	99.7	1	19168.3	0.C	
37 2H11/2 2	99.6	1	19198.9	0.C	
38 2H11/2 2	99.2	1	19223.8	0.C	
39 2H11/2 2	99.5	1	19250.2	0.C	
40 4F 7/2	99.8	1	20515.6	0.C	
41 4F 7/2	99.5	1	20563.8	0.C	
42 4F 7/2	99.5	1	20598.1	0.C	
43 4F 7/2	99.7	1	20665.4	0.C	

TABLE XV. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
 $\text{ErP}_5\text{O}_{14}$ (Cont'd)

FREE ION	PCT PURE	ZMU	THEO. ENERGY	EXP. ENERGY
44 4F 5/2	98.5	1	22210.3	0.0
45 4F 5/2	97.6	1	22222.8	0.0
46 4F 5/2	99.4	1	22258.3	0.0
47 4F 3/2	98.1	1	22527.0	0.0
48 4F 3/2	97.7	1	22615.0	0.0

TABLE XVI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
TmP₅O₁₄

TM IN TMP5O14. EXTERPOLATED BKM FROM COMPATIBLE NO AND EU HOMFS. 9/24/75.					
INIT.	8KM AND CENTRCIDS.	0 = -0.000			
-476.600	= B20	96.600 = B22	-93.700 = B40	329.000 = B42	333.600 = B42
181.100	= B60	-198.300 = B62	-222.500 = B62	262.700 = B64	-16.200 = B64
3H 6	255.0				
3F 4	5820.0	-264.000 = B44	-104.700 = B44		
3H 5	8435.0	269.100 = B66	65.300 = B66		
3H 4	12731.0				
3F 3	14529.0				
3F 2	15133.0				
1G 4	21325.0				
1D 2	27892.0				
FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY	
1 3H 6	100.0	0	-1.3	0.0	
2 3H 6	100.0	0	9.3	0.0	
3 3H 6	100.0	2	143.9	0.0	
4 3H 6	100.0	2	176.7	0.0	
5 3H 6	100.0	0	242.2	0.0	
6 3H 6	100.0	2	252.7	0.0	
7 3H 6	100.0	0	285.7	0.0	
8 3H 6	100.0	0	319.0	0.0	
9 3H 6	100.0	2	330.7	0.0	
10 3H 6	100.0	2	346.9	0.0	
11 3H 6	100.0	0	351.0	0.0	
12 3H 6	99.9	2	408.4	0.0	
13 3H 6	99.9	0	410.3	0.0	
14 3F 4	99.8	2	5691.8	0.0	
15 3F 4	99.6	0	5712.5	0.0	
16 3F 4	99.8	0	5779.7	0.0	
17 3F 4	99.7	2	5787.3	0.0	
18 3F 4	99.9	0	5827.5	0.0	
19 3F 4	99.9	2	5842.5	0.0	
20 3F 4	100.0	0	5874.3	0.0	
21 3F 4	99.9	0	5917.5	0.0	
22 3F 4	99.9	2	5927.4	0.0	
23 3H 5	100.0	2	8243.8	0.0	
24 3H 5	99.8	2	8251.2	0.0	
25 3H 5	99.7	0	8375.5	0.0	
26 3H 5	99.9	0	8379.6	0.0	
27 3H 5	99.9	2	8451.2	0.0	
28 3H 5	99.9	0	8471.6	0.0	
29 3H 5	99.9	2	8474.8	0.0	
30 3H 5	99.8	0	8513.7	0.0	
31 3H 5	99.9	2	8514.0	0.0	
32 3H 5	99.8	2	8554.2	0.0	
33 3H 5	99.9	0	8556.3	0.0	
34 3H 4	99.6	0	12547.4	0.0	
35 3H 4	100.0	0	12610.5	0.0	
36 3H 4	99.6	2	12671.9	0.0	
37 3H 4	99.6	0	12751.2	0.0	
38 3H 4	99.8	2	12757.8	0.0	
39 3H 4	99.8	2	12765.2	0.0	
40 3H 4	99.8	0	12792.7	0.0	
41 3H 4	99.6	2	12815.1	0.0	
42 3H 4	99.6	0	12830.0	0.0	
43 3F 3	99.3	0	14490.8	0.0	
44 3F 3	99.6	2	14494.9	0.0	
45 3F 3	99.3	0	14515.1	0.0	
46 3F 3	99.7	2	14534.1	0.0	
47 3F 3	99.3	0	14553.7	0.0	
48 3F 3	99.7	2	14559.2	0.0	
49 3F 3	99.5	2	14592.6	0.0	

TABLE XVI. ESTIMATED CRYSTAL FIELD PARAMETERS AND ENERGY LEVELS FOR
TmP₅O₁₄ (Cont'd)

FREE ION	PCT PURE	2MU	THEO. ENERGY	EXP. ENERGY
50 3F 2	99.2	0	15083.4	0.C
51 3F 2	99.6	2	15085.9	0.C
52 3F 2	99.2	2	15133.7	0.C
53 3F 2	99.6	0	15176.8	0.C
54 3F 2	99.8	0	15225.3	C.C
55 1G 4	100.0	2	21160.6	0.C
56 1G 4	100.0	0	21167.9	0.C
57 1G 4	100.0	0	21252.7	0.C
58 1G 4	100.0	2	21312.3	0.C
59 1G 4	100.0	0	21313.9	0.C
60 1G 4	100.0	2	21344.2	0.C
61 1G 4	100.0	0	21385.8	0.C
62 1G 4	100.0	0	21484.9	0.C
63 1G 4	100.0	2	21511.7	0.C
64 1D 2	100.0	0	27822.8	0.C
65 1D 2	100.0	2	27837.9	0.C
66 1D 2	100.0	2	27885.6	0.C
67 1D 2	100.0	0	27957.9	0.C
68 1D 2	100.0	0	27970.5	0.C

TABLE XVII. AMPLITUDES, A_{km} , IN $\text{CM}^{-1} \text{\AA}^{-k}$, OF SPHERICAL DECOMPOSITION OF LATTICE SUMS FOR $\text{NdP}_5\text{O}_{14}$ [†]

k	m	$A_{km} (q_0 = -1)^{\ddagger}$		$A_{km} (q_0 = -2)^{\ddagger}$	
		Real	Imaginary	Real	Imaginary
1	0	16797.4	0	23799.2	0
1	1	-37138.	5876.2	-69989.6	12348.9
2	0	-3006.66	0	-5414.44	0
2	1	24.0762	-210.429	32.735	-440.936
2	2	-46.2236	-699.385	-476.544	-742.301
3	0	146.631	0	272.599	0
3	1	113.903	-113.566	245.472	174.387
3	2	23.9621	118.058	23.3478	221.346
3	3	-107.	206.525	-512.996	235.769
4	0	1459.8	0	2659.56	0
4	1	-104.684	-153.643	-210.048	-308.525
4	2	-1196.65	985.944	-2418.41	1926.86
4	3	194.779	9.65227	400.361	21.1591
4	4	-658.119	-1337.65	-1156.92	-2600.78
5	0	-4.45292	0	-8.32774	0
5	1	759.959	-413.245	1502.53	-818.815
5	2	-33.9232	-12.0518	-69.3783	-25.2627
5	3	55.5247	-1357.2	124.874	-2646.4
5	4	74.1133	-34.314	148.632	-68.9808
5	5	-267.703	-218.441	-554.059	-448.519
6	0	202.617	0	403.34	0
6	1	2.44617	23.9365	5.33098	48.019
6	2	-95.8561	130.302	-189.637	258.726
6	3	-11.6831	-17.1279	-22.8872	-34.8373
6	4	-52.1825	-134.274	-116.977	-267.059
6	5	-12.6303	10.3804	-25.5546	20.0073
6	6	206.515	22.0685	411.215	43.7949
7	0	4.1059	0	8.26562	0
7	1	-47.8198	51.1209	-94.1572	101.206
7	2	-5.24923	-7.26414	-10.3708	-14.4391
7	3	-3.467	-15.118	-6.88997	-30.8619
7	4	4.838	1.1332	9.7122	2.29936
7	5	-25.74	-28.179	-51.1031	-56.7309
7	6	1.327	10.5704	2.61491	21.295
7	7	-32.06	20.2109	-64.6403	39.2683

[†]Lattice constants are $a = 8.771 \text{ \AA}$, $b = 9.012 \text{ \AA}$, $c = 13.057 \text{ \AA}$, and $\beta = 89.58 \text{ deg}$ (H. Y-P. Hong, Acta Crystallogr., B30 (1974), 468).

[‡]Oxygen charge, q_0 . Neodymium and phosphorus charges taken as $q_{Nd} = +3$, $q_P = -(3 + 14q_0)/5$.

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